# Malonic acid, 2,4-dimethylpent-3-yl propyl ester

**Inchi:** InChI=1S/C13H24O4/c1-6-7-16-11(14)8-12(15)17-13(9(2)3)10(4)5/h9-10,13H,6-8H2,1-5

**InchiKey:** XYGLQRLIVIQKAJ-UHFFFAOYSA-N

**Formula:** C13H24O4

**SMILES:** CCCOC(=O)CC(=O)OC(C(C)C)C(C)C

**Mol. weight [g/mol]:** 244.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -416.58 | kJ/mol | Joback Method |
| hf | -817.09 | kJ/mol | Joback Method |
| hfus | 24.43 | kJ/mol | Joback Method |
| hvap | 61.68 | kJ/mol | Joback Method |
| log10ws | -2.62 | | Crippen Method |
| logp | 2.554 | | Crippen Method |
| mcvol | 208.910 | ml/mol | McGowan Method |
| pc | 1810.77 | kPa | Joback Method |
| rinpol | 1489.00 | | NIST Webbook |
| rinpol | 1489.00 | | NIST Webbook |
| tb | 648.10 | K | Joback Method |
| tc | 832.83 | K | Joback Method |
| tf | 335.59 | K | Joback Method |
| vc | 0.793 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 569.70 | J/mol×K | 648.10 | Joback Method |
| cpg | 641.76 | J/mol×K | 802.04 | Joback Method |
| cpg | 628.87 | J/mol×K | 771.25 | Joback Method |
| cpg | 615.23 | J/mol×K | 740.46 | Joback Method |
| cpg | 600.82 | J/mol×K | 709.68 | Joback Method |
| cpg | 585.64 | J/mol×K | 678.89 | Joback Method |
| cpg | 653.89 | J/mol×K | 832.83 | Joback Method |
| dvisc | 0.0001087 | Pa×s | 648.10 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001499 | Pa×s | 596.02 | Joback Method |
| dvisc | 0.0002198 | Pa×s | 543.93 | Joback Method |
| dvisc | 0.0003497 | Pa×s | 491.85 | Joback Method |
| dvisc | 0.0006210 | Pa×s | 439.76 | Joback Method |
| dvisc | 0.0012868 | Pa×s | 387.68 | Joback Method |
| dvisc | 0.0033428 | Pa×s | 335.59 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U349009&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |